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# Wiener index of hexagonal chains under some transformations

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**Abstract:** The Wiener index is a topological index of a molecule, defined as the sum of distances between all pairs of vertices in the chemical graph. Hexagonal chains consist of hexagonal rings connected with each other by edges. This class of chains contains molecular graphs of unbranched catacondensed benzenoid hydrocarbons. A segment of length  $\ell$  of a chain is its maximal subchain with  $\ell$  linear annelated hexagons. We consider chains in which all segments have equal lengths. Such chains can be uniquely represented by binary vectors. The Wiener index of hexagonal chains under some operations on the corresponding binary vectors are investigated. The obtained results may be useful in studying of topological indices for sets of hexagonal chains induced by algebraic constructions.

**Keywords:** Topological index, Wiener index, hexagonal chain.

**MSC:** 05C30, 92E10

## 1. Introduction

**D**istance-based graph invariants, called topological indices, are widely used in studying of structure of molecular graphs in organic chemistry. The Wiener index is a well-known topological index introduced as structural descriptor for acyclic organic molecules [1]. It is defined as the sum of distances between all unordered pairs of vertices of an undirected connected graph  $G$  with vertex set  $V(G)$ :

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v),$$

where distance  $d(u,v)$  is the number of edges in the shortest path connecting vertices  $u$  and  $v$  in  $G$ . The Wiener index is intensively studied in mathematical and theoretical chemistry and has found numerous applications in the modeling of physico-chemical, pharmacological and biological properties of organic molecules (see books [2–10] and reviews [11–19]).

We will consider the Wiener index of hexagonal chains that include molecular graphs of catacondensed unbranched benzenoid hydrocarbons. Since this class of chemical compounds is attracting the great attention of theoretical chemists, the theory of the Wiener index of the respective molecular graphs has been developed for many years [20,21]. Changes of the Wiener index of polycyclic structures under transformations of various kinds were investigated in [22–29]. The structure of hexagonal chains of certain classes can be encoded by binary vectors. Operations on chains' binary codes generate new hexagonal chains. In this paper, relations between Wiener indices of chains for some operations on chains' codes are studied and illustrative numeric examples are presented.

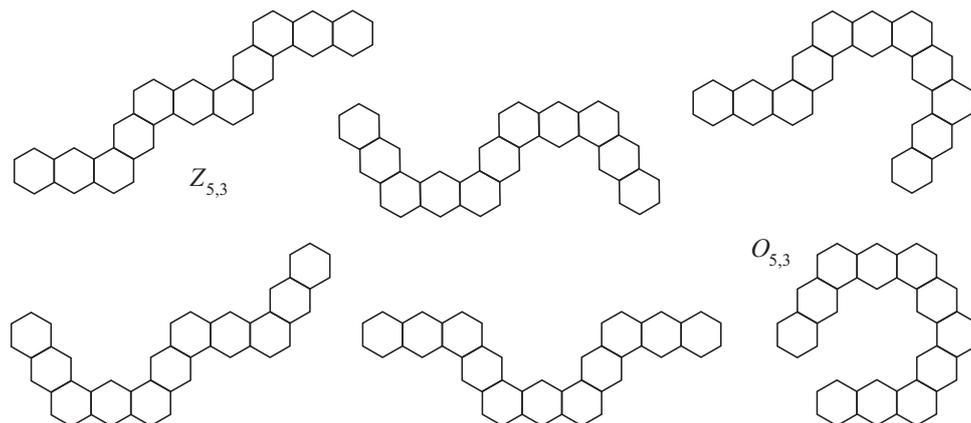


Figure 1. All hexagonal chains of  $\mathcal{G}_{5,3}$  with 5 segments of length 3.

### 2. Hexagonal chains and their segments

The classification of molecular graphs of benzenoid hydrocarbons is based on the kind of connection of hexagonal rings with one another [30]. A hexagonal chain is a connected plane graph in which every inner face is bounded by a hexagon. An inner face with its hexagonal bound is called a *hexagonal ring* (or simply *ring*). Two hexagonal rings of a chain are either disjoint or have exactly one common edge (adjacent rings), and no three rings share a common vertex. A ring having exactly one adjacent ring is called *terminal*. A hexagonal chain has exactly two terminal rings. A ring adjacent to exactly two other rings has two vertices of degree 2. If these two vertices are adjacent, then the ring is angularly connected; if these two vertices are not adjacent, then it is linearly connected. A *segment* is a maximal subchain in which all rings are linearly connected. A segment including a terminal hexagon is a *terminal segment*. The number of hexagons in a segment is called its *length*. Denote by  $\mathcal{G}_{n,\ell}$  the set of all hexagonal chains having  $n$  segments of length  $\ell$ . All hexagonal chains of  $\mathcal{G}_{5,3}$  are shown in Figure 1. Some properties of graphs of this class were studied in [31–35]. Hexagonal chains of  $\mathcal{G}_{n,2}$  with minimal length of segments are known as fibonacenes [36,37]. The number of hexagonal rings of  $G \in \mathcal{G}_{n,\ell}$  is equal to  $h = n(\ell - 1) + 1$  and the number of segments is  $n = (h - 1)/(\ell - 1)$ . Since  $|\mathcal{G}_{n,2}| = |\mathcal{G}_{n,\ell}|$  for all  $\ell \geq 3$ , the cardinality of  $\mathcal{G}_{n,\ell}$  is equal to  $|\mathcal{G}_{n,\ell}| = 2^{n-3} + 2^{\lfloor \frac{n-3}{2} \rfloor}$ ,  $n \geq 2$  [37].

### 3. Representation of hexagonal chains

The structure of hexagonal chains is completely defined by a way of segment attachment. We consider a nonterminal segment  $S$  with two neighboring segments embedded into the regular hexagonal lattice on the plane and draw a line through the centers of the hexagons of  $S$ . If the neighboring segments of  $S$  lie on different sides of the line, then  $S$  is called a *zigzag* segment. If these segments lie on the same side, then  $S$  is said to be a *spiral* segment. It is convenient to assume that the terminal segments are zigzag segments. For a hexagonal chain  $X$ , denote by  $U(X)$  the set of its spiral segments,  $u_X = |U(X)|$ .

Based on two types of segments, hexagonal chains of  $\mathcal{G}_{n,\ell}$  can be represented by binary codes. We assume that all segments of a chain are sequentially numbered by  $0, 1, \dots, n - 1$  beginning from a terminal segment. Since the terminal segments can be ignored when a chain is restored, codes of all hexagonal chains of  $\mathcal{G}_{n,\ell}$  have a length of  $n - 2$ ,  $n \geq 3$ . Assume that every spiral segment of chain  $X$  corresponds to 1 in the code of  $X$  while every zigzag segment corresponds to 0. A binary code of hexagonal chain  $X$  and a hexagonal chain  $X$  induced by a binary word  $r$  will be denoted by  $r(X)$  and  $X(r)$ , respectively. Note that molecular graphs of more general classes of benzenoid hydrocarbons can be also represented by binary codes [31,38].

There are two extremal chains with respect to the type of segments. The *zigzag* hexagonal chain  $Z_{n,\ell} \in \mathcal{G}_{n,\ell}$  contains only zigzag segments,  $r(Z_{n,\ell}) = (00..0)$ . All segments of the *spiral* hexagonal chain  $O_{n,\ell} \in \mathcal{G}_{n,\ell}$  are spiral ones (with the exception of the terminal segments),  $r(O_{n,\ell}) = (11..1)$ . The zigzag and the spiral hexagonal chains of  $\mathcal{G}_{5,3}$  are shown in Figure 1. Denote by  $e_i$  the binary vector  $e_i = (0..01^i..0)$  of length  $n - 2$  for  $n \geq 3, i = 1, 2, \dots, n - 2$ . These vectors form the standard basis for the vector space of dimension  $n - 2$  over  $\mathbb{Z}_2$ . Let  $C_i$  be the basis hexagonal chains corresponding to basis vectors  $e_i, i = 1, 2, \dots, n - 2$ . Then code  $r(X)$  of

$X \in \mathcal{G}_{n,\ell}$  can be expressed as a linear combination of the basis vectors:  $r(X) = x_1 e_1 + x_2 e_2 + \dots + x_{n-2} e_{n-2}$ . Since codes  $e_i$  and  $e_{n-i-1}$  are symmetrical, basis chains  $C_i$  and  $C_{n-i-1}$  are isomorphic and  $W(C_i) = W(C_{n-i-1})$ .

Hexagonal chains  $O_{n,\ell}$  and  $Z_{n,\ell}$  are extremal graphs with respect to the Wiener index among all chains of  $\mathcal{G}_{n,\ell}$  [13]:  $W(O_{n,\ell}) < W(G) < W(Z_{n,\ell})$  for all  $G \in \mathcal{G}_{n,\ell} \setminus \{O_{n,\ell}, Z_{n,\ell}\}$ , where

$$\begin{aligned} W_{\min} &= (8n^3(\ell - 1)^2(2\ell - 3) + 96n^2(\ell - 1)^2 - 2n(\ell - 1)(2\ell - 75) + 81) / 3, \\ W_{\max} &= (16n^3(\ell - 1)^3 + 72n^2(\ell - 1)^2 + n(\ell - 1)(12\ell + 134) + 81) / 3. \end{aligned}$$

The average of these extremal values is equal to

$$\begin{aligned} W_{\text{avr}} &= (W_{\min} + W_{\max}) / 2 \\ &= (4n^3(\ell - 1)^2(4\ell - 5) + 84n^2(\ell - 1)^2 + 2n(\ell - 1)(2\ell + 71) + 81) / 3. \end{aligned}$$

#### 4. Graph operations

Let  $X, Y \in \mathcal{G}_{n,\ell}$  with codes  $r(X) = x = (x_1, x_2, \dots, x_{n-2})$  and  $r(Y) = y = (y_1, y_2, \dots, y_{n-2})$ . Define the following operations of these hexagonal chains:

- the complement of a hexagonal chain  $X$  is a new chain  $Y$  with code  $r(Y) = r(\bar{X}) = (\bar{x}_1, \bar{x}_2, \dots, \bar{x}_{n-2})$ , that is,  $r(Y)$  is a bitwise complement of  $r(X)$ . This operation changes the type of all segments of  $X$ . Example:  $(10011) = (01100)$ ;
- the unary operation  $t_{i,j}(X)$  changes the type of  $i$ -th and  $j$ -th segments to opposite. For example, if  $r(X) = (1000111)$ , then hexagonal chain  $Y = t_{2,6}(X)$  has code  $r(Y) = (1100101)$ ;
- the sum modulo 2 of hexagonal chains  $X$  and  $Y$  is a new chain  $G = X + Y$  with code  $r(G) = x + y = (x_1 + y_1, x_2 + y_2, \dots, x_{n-2} + y_{n-2})$ . The resulting chain inherits spiral segments of the initial chains except spiral segments in the same positions. Example:  $(10011) + (10101) = (00110)$ ;
- the difference modulo 2 of hexagonal chains  $X$  and  $Y$  is a new chain  $G = X - Y$  with code  $r(G) = x - y = (x_1 - y_1, x_2 - y_2, \dots, x_{n-2} - y_{n-2})$ . Despite of  $G = X - Y = X + Y$ , we will distinguish between these operations. Example:  $(10011) - (10101) = (00110)$ ;
- a hexagonal chain  $G = XY$  is called the product of chains  $X$  and  $Y$  with code  $r(G) = xy = (x_1y_1, x_2y_2, \dots, x_{n-2}y_{n-2})$ . This operation is an analogue of bitwise logical operation "AND". The resulting chain has spiral segments if they are in the same positions of the initial chains. Example:  $(10011)(10101) = (10001)$ ;
- operation " $\vee$ " of hexagonal chains  $X$  and  $Y$  gives a new chain  $G = X \vee Y$  with code  $r(G) = x \vee y = (x_1 \vee y_1, x_2 \vee y_2, \dots, x_{n-2} \vee y_{n-2})$ , where  $x_i \vee y_i$  is an analogue of bitwise logical operation "OR". All spiral segments of the initial chains are served in  $G$ . Example:  $(10011) \vee (10101) = (10111)$ .

The binary relation  $X \leq Y$  between chains  $X, Y \in \mathcal{G}_{n,\ell}$  is defined by conditions  $x_i \leq y_i, i = 1, 2, \dots, n - 2$ . This relation induces a partial order on  $\mathcal{G}_{n,\ell}$ .

In the next section, changes of the Wiener index under introduced operations over chains' codes are examined.

#### 5. Changes of the Wiener index

The following useful formula allows the calculation Wiener index of hexagonal chains through their binary codes [26].

**Proposition 1.** For a hexagonal chain  $X \in \mathcal{G}_{n,\ell}$  with a code  $(x_1, x_2, \dots, x_{n-2})$ ,

$$W(X) = W_{\max} - 16(\ell - 1)^2 \sum_{i=1}^{n-2} i(n - i - 1)x_i.$$

The sum of Wiener indices of a hexagonal chain and its complement is twice the average value  $W_{\text{avr}}$ .

**Proposition 2.** If  $X \in \mathcal{G}_{n,\ell}$ , then  $W(\bar{X}) = W_{\min} + W_{\max} - W(X)$ .

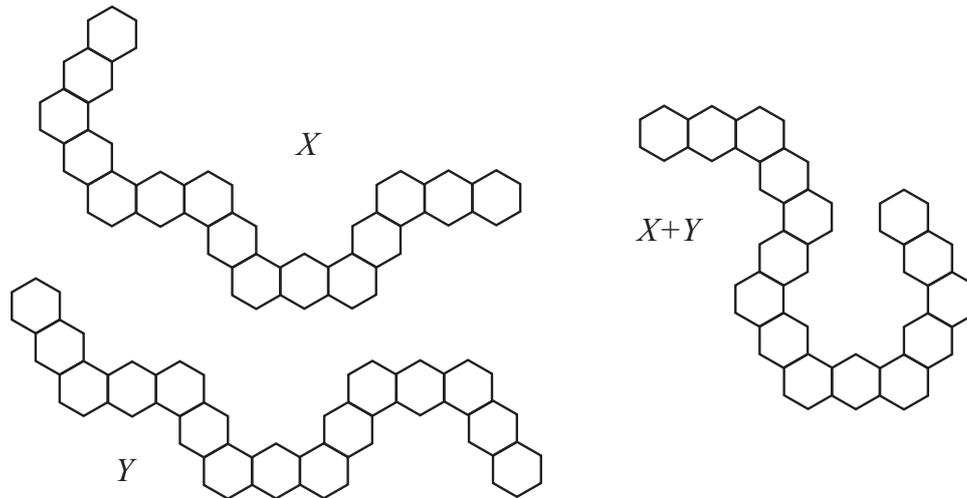


Figure 2. Hexagonal chains  $X, Y \in \mathcal{G}_{7,3}$  and  $X + Y$ .

**Proof.** By Proposition 1,

$$\begin{aligned} W(X) + W(\bar{X}) &= W_{\max} + W_{\max} - 16(\ell - 1)^2 \sum_{i=1}^{n-2} i(n - i - 1) \cdot 1 \\ &= W_{\max} + W_{\min}. \end{aligned}$$

□

Proposition 2 allows to determine the structure of hexagonal chains with average value of the Wiener index. If  $r(X) = r(\bar{X})$ , then chains  $X$  and  $\bar{X}$  are obviously isomorphic. This implies equality  $W(X) = W_{\text{avr}}$ . There are also non-isomorphic chains  $X$  and  $\bar{X}$  with property  $W(X) = W(\bar{X}) = W_{\text{avr}}$  [26].

Consider hexagonal chains without units in the same positions of their codes.

**Proposition 3.** Let  $X, Y \in \mathcal{G}_{n,\ell}$  and  $XY = Z_{n,\ell}$ . If  $G = X + Y$ , then

$$W(G) = W(X) + W(Y) - W_{\max}.$$

**Proof.** Let  $x = r(X)$  and  $y = r(Y)$ . By Proposition 1, we can write

$$W(X) + W(Y) - W_{\max} = W_{\max} - 16(\ell - 1)^2 \sum_i i(n - i - 1)(x_i + y_i) = W(G).$$

□

As an illustration, consider chains  $X, Y \in \mathcal{G}_{7,3}$  and  $G = X + Y$  shown in Figure 2. These graphs have codes  $r(X) = (10010)$ ,  $r(Y) = (00101)$ , and  $r(G) = (10111)$ . By computer calculations, their Wiener indices are  $W(X) = 19327$ ,  $W(Y) = 19263$ ,  $W(G) = 18431$ , and  $W_{\max} = 20159$ . By Proposition 3,  $W(G) = 19327 + 19263 - 20159 = 18431$ .

**Proposition 4.** Let  $X, Y \in \mathcal{G}_{n,\ell}$  and  $Y \leq X$ . If  $G = X - Y$ , then

$$W(G) = W(X) - W(Y) + W_{\max}.$$

**Proof.** If  $x = r(X)$  and  $y = r(Y)$ , then by Proposition 1

$$\begin{aligned} W(Y) - W(X) - W_{\max} &= -W_{\max} + 16(\ell - 1)^2 \sum_i i(n - i - 1)(x_i - y_i) \\ &= -W(G). \end{aligned}$$

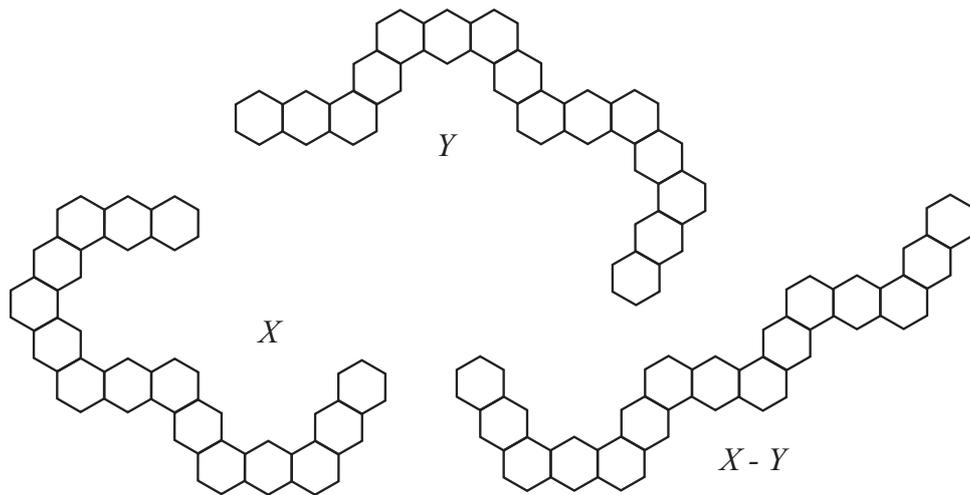


Figure 3. Hexagonal chains  $X, Y \in \mathcal{G}_{7,3}$  and  $X - Y$ .

Since  $y_i \leq x_i, (x_i - y_i) \geq 0$  for every  $i$ . □

Hexagonal chains  $X, Y \in \mathcal{G}_{7,3}$  and  $G = X - Y$  shown in Figure 3 illustrate Proposition 4. Codes of these graphs are  $r(X) = (11001), r(Y) = (01001)$ , and  $r(G) = (10000)$ . Computer calculations give the following Wiener indices:  $W(X) = 19007, W(Y) = 19327$ , and  $W(G) = 19839$ . By Proposition 4,  $W(G) = 19007 - 19327 + 20159 = 19839$ .

The next result answers on the following question: how many times do we need to apply operation  $t_{i,j}$  to a hexagonal chain  $X$  such that  $W(X) = W(t_{i,j}(X))$ ? For asymmetrical chains, it is sufficient to apply the operation once time.

**Corollary 1.** Let  $X \in \mathcal{G}_{n,\ell}$  be an asymmetrical hexagonal chain with a code  $(x_1, x_2, \dots, x_{n-2})$ , i.e.,  $x_i \neq x_{n-i-1}$  for some  $i \in \{1, 2, \dots, \lceil (n-2)/2 \rceil\}$ . If  $Y = t_{i,n-i-1}(X)$ , then  $W(Y) = W(X)$ .

**Proof.** Assume that  $x_i = 0$  and  $x_{n-i-1} = 1$ . Then  $Y = (X + C_i) - C_{n-i-1}$ . By Propositions 4 and 3, we can write  $W(Y) = W(X + C_i) - W(C_{n-i-1}) + W_{\max} = W(X) + W(C_i) - W_{\max} - W(C_{n-i-1}) + W_{\max} = W(X)$ . □

Let  $\mu(X)$  be the number of pairs of non-equal  $i$ -th and  $(n - i - 1)$ -th components of chain's code  $r(X)$ ,  $i = 1, 2, \dots, \lceil (n - 2)/2 \rceil$ . Repeating Corollary 1, one can construct a family of  $2^{\mu(X)}$  chains having the same Wiener index (some chains may be isomorphic).

Decomposition of the Wiener index of chains of  $\mathcal{G}_{n,\ell}$  into the sum of Wiener indices of basis hexagonal chains was reported in [26]. It can be also derived using graph operations.

**Corollary 2.** Let  $X \in \mathcal{G}_{n,\ell}$  and  $r(X) = (x_1, x_2, \dots, x_{n-2})$ . Then

$$W(X) = x_1W(C_1) + x_2W(C_2) + \dots + x_{n-2}W(C_{n-2}) - (u - 1)W_{\max},$$

where  $u = x_1 + x_2 + \dots + x_{n-2}$  is the number of units of  $x$ .

**Proof.** Let  $i_1, i_2, \dots, i_u$  be positions of units in  $x$ . Then the corresponding hexagonal chain  $X$  can be represented as  $X = C_{i_1} + C_{i_2} + \dots + C_{i_u}$ . Applying Proposition 3, we get  $W(X) = W(C_{i_1}) + W(C_{i_2}) + \dots + W(C_{i_u}) - (u - 1)W_{\max} = x_1W(C_1) + x_2W(C_2) + \dots + x_{n-2}W(C_{n-2}) - (u - 1)W_{\max}$ . □

Let us consider operations of hexagonal chains with arbitrary codes.

**Proposition 5.** Let  $X, Y \in \mathcal{G}_{n,\ell}$ . If  $G = X + Y$ , then

$$W(G) = W(X) + W(Y) - 2W(XY) + W_{\max}.$$

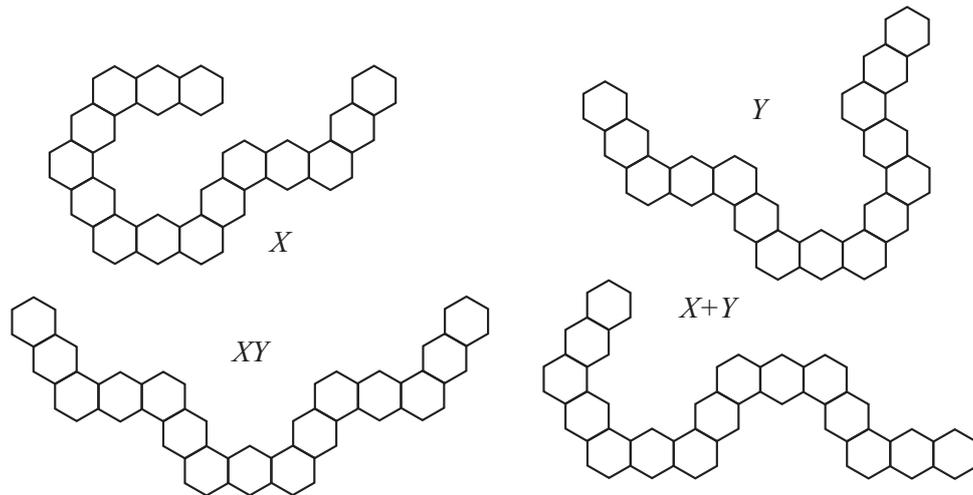


Figure 4. Hexagonal chains  $X, Y \in \mathcal{G}_{7,3}$  and  $X + Y$  (general case).

**Proof.** It is easy to verify that the hexagonal chain  $G$  can be represented as  $G = X + Y = (X - XY) + (Y - XY)$ , where  $(X - XY)(Y - XY) = Z_{n,\ell}$  and  $X \geq XY, Y \geq XY$ . By Propositions 3 and 4,

$$\begin{aligned} W(G) &= W(X - XY) + W(Y - XY) - W_{\max} \\ &= W(X) - W(XY) + W_{\max} + W(Y) - W(XY) + W_{\max} - W_{\max} \\ &= W(X) + W(Y) - 2W(XY) + W_{\max}. \end{aligned}$$

□

Hexagonal chains  $X, Y \in \mathcal{G}_{7,3}$  and  $G = X + Y$  shown in Figure 4 illustrate Proposition 5. These chains have codes  $r(X) = (11100), r(Y) = (00110), r(XY) = (00100)$ , and  $r(G) = (11010)$ . Their Wiener indices are  $W(X) = 18751, W(Y) = 19071, W(XY) = 19583$ , and  $W(G) = 18815$ . By applying Proposition 5,  $W(G) = 18751 + 19071 - 2 \cdot 19583 + 20159 = 18815$ .

**Proposition 6.** Let  $X, Y \in \mathcal{G}_{n,\ell}$ . If  $G = X - Y$ , then

$$W(G) = W(X) - W(Y) + 2W(\overline{XY}) - W_{\max}.$$

**Proof.** Hexagonal chain  $G$  can be decomposed as  $G = X - Y = (X + \overline{XY}) - (Y - \overline{XY})$ , where  $(X + \overline{XY}) \geq (Y - \overline{XY}), X(\overline{XY}) = Z_{n,\ell}$  and  $Y \geq \overline{XY}$ . By Propositions 3 and 4,

$$\begin{aligned} W(G) &= W(X + \overline{XY}) - W(Y - \overline{XY}) + W_{\max} \\ &= W(X) + W(\overline{XY}) - W_{\max} - (W(Y) - W(\overline{XY}) + W_{\max}) + W_{\max} \\ &= W(X) - W(Y) + 2W(\overline{XY}) - W_{\max}. \end{aligned}$$

□

Consider again hexagonal chains  $X$  and  $Y$  shown in Figure 4. Chains  $\overline{XY}$  and  $X - Y$  have codes  $r(\overline{XY}) = (00010), r(X - Y) = (00101)$ , and Wiener indices  $W(\overline{XY}) = 19647, W(X - Y) = 18815$ . By Proposition 6, we obtain  $W(G) = 18751 - 19071 + 2 \cdot 19647 - 20159 = 18815$ .

**Proposition 7.** Let  $X, Y \in \mathcal{G}_{n,\ell}$ . If  $G = X \vee Y$ , then

$$W(G) = W(X) + W(Y) - W(XY).$$

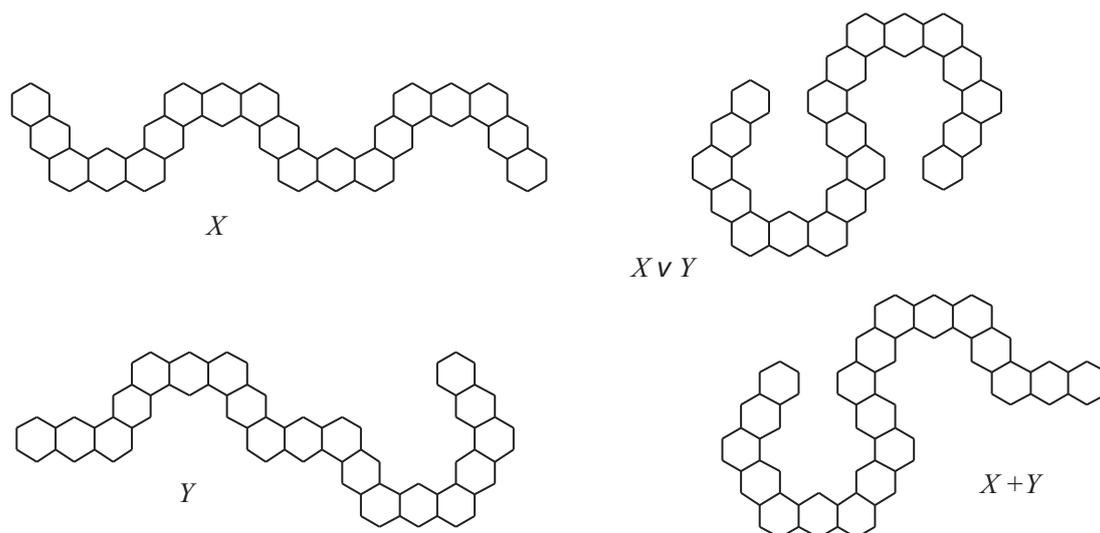


Figure 5. Hexagonal chains  $X, Y \in \mathcal{G}_{9,3}$  and  $X \vee Y$ .

**Proof.** Using Proposition 1, we get

$$W(X) + W(Y) - W(XY) = W_{\max} - 16(\ell - 1)^2 \sum_i i(n - i - 1)(x_i + y_i - x_i y_i),$$

$$W(X \vee Y) = W_{\max} - 16(\ell - 1)^2 \sum_i i(n - i - 1)(x_i \vee y_i).$$

Comparison of these equalities completes the proof.  $\square$

Hexagonal chains  $X, Y \in \mathcal{G}_{9,3}$  and  $G = X \vee Y$  of Figure 5 illustrate Proposition 7. The structure of graph  $X + Y$  is presented for comparison. These chains have codes  $r(X) = (1010101)$ ,  $r(Y) = (0100011)$ ,  $r(XY) = (0000001)$ , and  $r(G) = (1110111)$ , and their Wiener indices are equal to  $W(X) = 37111$ ,  $W(Y) = 37943$ ,  $W(XY) = 39479$ , and  $W(G) = 35575$ . By Proposition 7,  $W(G) = 37111 + 37943 - 39479 = 35575$ .

In conclusion, we note that the considered approach may be useful in studying of topological indices for sets of hexagonal chains induced by algebraic constructions.

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## References

- [1] Wiener, H. (1947). Structural determination of paraffin boiling points. *Journal of the American Chemical Society*, 69, 17–20.
- [2] Dehmer, M., & Emmert-Streib, F. (Eds.) (2014). *Quantitative Graph Theory: Mathematical Foundations and Applications*. Discrete Mathematics and Its Applications. Chapman and Hall/CRC.
- [3] Devillers, J., & Balaban, A. T. (Eds.) (1999). *Topological Indices and Related Descriptors in QSAR and QSPR*. Reading: Gordon & Breach.
- [4] Diudea, M. V. (Ed.) (2001). *QSPR/QSAR Studies by Molecular Descriptors*. Huntington, New York: Nova.
- [5] Gutman, I., & Polansky, O. E. (1986). *Mathematical Concepts in Organic Chemistry*. Berlin: Springer-Verlag.
- [6] Gutman, I., & Furtula, B. (Eds.) (2012). *Distance in Molecular Graphs — Theory*. Mathematical Chemistry Monographs, 12, University of Kragujevac, Kragujevac, Serbia.
- [7] Gutman, I., & Furtula, B. (Eds.) (2012). *Distance in Molecular Graphs — Applications*. Mathematical Chemistry Monographs, 13, University of Kragujevac, Kragujevac, Serbia.
- [8] Rouvray, D. H., & King, R. B. (Eds.) (2002). *Topology in Chemistry. Discrete Mathematics of Molecules*. Woodhead Publishing.

- [9] Todeschini, R., & Consonni, V. (2000). *Handbook of Molecular Descriptors*. Weinheim: Wiley-VCH.
- [10] Trinajstić, N. (1992). *Chemical Graph Theory*. Boca Raton: CRC Press.
- [11] Balaban, A. T., Motoc, I., Bonchev, D., & Mekenyan, O. (1983). Topological indices for structure-activity correlations. *Topics in Current Chemistry*, 114, 21–55.
- [12] Dobrynin, A. A., Entringer, R., & Gutman, I. (2001). Wiener index for trees: theory and applications. *Acta Applicandae Mathematicae*, 66(3), 211–249.
- [13] Dobrynin, A. A., Gutman, I., Klavžar, S., & Žigert, P. (2002). Wiener index of hexagonal systems. *Acta Applicandae Mathematicae*, 72(3), 247–294.
- [14] Entringer, R. C. (1997). Distance in graphs: trees. *Journal of Combinatorial Mathematics and Combinatorial Computing*, 24, 65–84.
- [15] Gutman, I., & Potgieter, J. H. (1997). Wiener index and intermolecular forces. *Journal of the Serbian Chemical Society*, 62, 185–192.
- [16] Knor, M., Škrekovski, R., & Tepeh, A. (2016). Mathematical aspects of Wiener index. *Ars Mathematica Contemporanea*, 11(2), 327–352.
- [17] Nikolić, S., Trinajstić, N., & Mihalić, Z. (1995). The Wiener index: developments and applications. *Croatica Chemica Acta*, 68, 105–129.
- [18] Rouvray, D. H. (1983). Should we have designs on topological indices? In: King, R.B. (Ed.), *Chemical Application of Topology and Graph Theory* (pp. 159–177). Studies in Physical and Theoretical Chemistry, 28. Amsterdam: Elsevier.
- [19] Rouvray, D. H. (1987). The modeling of chemical phenomena using topological indices. *Journal of Computational Chemistry*, 8, 470–480.
- [20] Gutman, I. (1992). Topological properties of benzenoid systems. *Topics in Current Chemistry*, 162, 21–28.
- [21] Gutman, I., & Cyvin, S. J. (1989). *Introduction to the Theory of Benzenoid Hydrocarbons*. Berlin: Springer-Verlag.
- [22] Bonchev, D., Mekenyan, O., & Trinajstić, N. (1980). Topological characterization of cyclic structures. *Journal of Quantum Chemistry*, 17(5), 845–893.
- [23] Dobrynin, A. A. (1988). The distance of graphs of cata-condensed hexagonal polycyclic systems during their transformations. *Vychisl. Sistemy*, 127, 3–39, in Russian.
- [24] Dobrynin, A. A. (1998). Formula for calculating the Wiener index of catacondensed benzenoid graphs. *Journal of Chemical Information and Computer Sciences*, 38(5), 811–814.
- [25] Dobrynin, A. A. (2003). Wiener index decomposition based on vertex degrees of catacondensed benzenoid graphs. *MATCH Communications in Mathematical and in Computer Chemistry*, 49, 37–46.
- [26] Dobrynin, A. A. (2014). Wiener index of hexagonal chains with segments of equal length. In: Dehmer, M., & Emmert-Streib, F. (Eds.), *Quantitative Graph Theory: Mathematical Foundations and Applications* (pp. 81–109). Discrete Mathematics and Its Applications. Chapman and Hall/CRC.
- [27] Polansky, O. E., & Bonchev, D. (1986). The Wiener number of graphs. I. General theory and changes due to some graph operations. *MATCH Communications in Mathematical and in Computer Chemistry*, 21, 133–186.
- [28] Polansky, O. E., & Bonchev, D. (1990). Theory of the Wiener number of graphs. II. Transfer graphs and some of their metric properties. *MATCH Communications in Mathematical and in Computer Chemistry*, 25, 3–39.
- [29] Xu, L., & Guo, X. (2006). Catacondensed hexagonal systems with large Wiener numbers. *MATCH Communications in Mathematical and in Computer Chemistry*, 55, 137–158.
- [30] Trinajstić, N. (1990). On the classification of polyhex hydrocarbons. *Journal of Mathematical Chemistry*, 5(2), 171–175.
- [31] Jovanovic, A.D. (1988). Combinatorial characterization of hexagonal systems. *Discrete Applied Mathematics*, 19(1–3), 259–270.
- [32] Dobrynin, A. A. (2010). On the Wiener index of fibonacenes. *MATCH Communications in Mathematical and in Computer Chemistry*, 64(3), 707–726.
- [33] Dobrynin, A. A. (2013). On the Wiener index of certain families of fibonacenes. *MATCH Communications in Mathematical and in Computer Chemistry*, 70(2), 565–574.
- [34] Dobrynin, A. A. (2017). Hexagonal chains with segments of equal lengths having distinct sizes and the same Wiener index. *MATCH Communications in Mathematical and in Computer Chemistry*, 78(1), 121–132.
- [35] Dobrynin, A. A., & Estaji, E. (2019). Wiener index of certain families of hexagonal chains. *Journal of Applied Mathematics and Computing*, 59(1–2), 245–256.
- [36] Gutman, I., & Klavžar, S. (2006). Chemical graph theory of fibonacenes. *MATCH Communications in Mathematical and in Computer Chemistry*, 55, 39–54.
- [37] Balaban, A. T. (1989). Chemical graphs. Part 50. Symmetry and enumeration of fibonacenes (unbranched catacondensed benzenoids isoarithmic with helicenes and zigzag catafusenes). *MATCH Communications in Mathematical and in Computer Chemistry*, 24, 9–38.

- [38] Herndon, W. C., & Bruce, A. J. (1987). Perimeter codes for benzenoid aromatic hydrocarbons. In: King, R. B., & Rouvray, D. H. (Eds.), *Graph Theory and Topology in Chemistry* (pp. 491–513). Studies in Physical and Theoretical Chemistry, 51. Amsterdam: Elsevier.



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